

Electronic structure of multiquantum giant vortex states in mesoscopic superconducting disks

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We report self-consistent calculations of the microscopic electronic structure of the so-called giant vortex states. These novel multiquantum vortex states, detected by recent magnetization measurements on submicron disks, are qualitatively different from the Abrikosov vortices in the bulk. We find that, in addition to multiple branches of bound states in the core region, the local tunneling density of states exhibits Tomasch oscillations due to the single-particle interference arising from quantum confinement. These features should be directly observable by scanning tunneling spectroscopy.

74.20.Fg, 74.80.-g, 73.20.-r

I. INTRODUCTION

Superconducting vortices are topological singularities in the order parameter [1]. In a bulk system each vortex carries a single flux quantum, while vortices with multiple flux quanta are not favorable energetically [2]. In small superconductors, however, the situation may be different. Today's nanotechnology can provide valuable insight into the nature of mesoscopic superconductors, whose linear dimensions can be comparable to the coherence length or the inter-vortex distance of the Abrikosov lattice. The following question then arises naturally: does single-quantum vortex matter survive the limit of decreasing sample size? More than thirty years ago, Fink and Presson gave the intriguing answer "not always" in their pioneering work [3] on a related system: a thin cylinder in parallel field. They have shown it theoretically, within the framework of the phenomenological Ginzburg-Landau (GL) theory, and also provided experimental evidence [4] for the existence of an enormous superfluid eddy current on the surface of a thin cylinder. They called this state a giant vortex state. While the work of Fink and Presson was largely forgotten for the next several decades, it nevertheless anticipated the present excitement in the field of nanoscale superconductivity. With recent advances in the controlled fabrication and study of nanometer-scale superconductors, the concept of giant vortex has been brought back to focus by Moshchalkov and coworkers a few years ago [5]. Their experiments on mesoscopic squares and square rings have indeed revealed that small superconductors do not always favor many-vortex states reminiscent of the Abrikosov vortex lattice. The measured H - T phase boundaries of these small structures were explained in terms of giant vortex states in the GL picture [5]. Subsequent experiments on submicron disks [6] have further shown the existence of

giant vortex states inside the phase boundaries. Within the GL framework [6–10] some of the abrupt changes in the magnetization observed have been attributed, e.g., to the collapse of a multi-vortex state into a giant vortex, or to transitions among different giant vortex states.

This new phase of vortex matter has a single vortex occupying the sample, carrying multiple fluxoid [3,11,12] quanta. Such a state has no immediate analogue in bulk systems, and would only be similar to vortex states predicted for artificially patterned structures [13,14]. Moshchalkov *et al.* [15] have also suggested that giant vortex states can cause the peculiar paramagnetic Meissner effect seen in granular and mesoscopic superconductors [16,17], through the compression of the flux trapped in the sample. This effect has been seen experimentally in mesoscopic systems by Geim and coworkers [18]. As it is apparent from these recent experiments, mesoscopic superconductors exhibit novel quantum phenomena that are not observable in bulk systems. Studying their unique properties is crucial not only for potential applications but also for better understanding of nanoscale superconductivity.

Despite the fact that the existence of giant vortex states has been indicated more than three decades ago, and that their counterpart in nanoscale superconductors has been under intense scrutiny in recent years, there has been no microscopic, self-consistent theoretical study of its electronic structure. In this paper we report the results of such a microscopic and self-consistent study of multiquantum giant vortex states in s -wave superconducting disks of submicron size,* using the Bogoliubov-de

*After the completion of this work, we became aware of the recent results of A. S. Mel'nikov and V. M. Vinokur [19], in which the possible application of mesoscopic disks as quantum

Gennes (BdG) formalism [11]. The spectroscopic properties we have obtained for such vortex states can be probed directly by scanning tunneling microscopy (STM). Although GL studies give a good qualitative picture for a wide range of parameters, quantitatively reliable results are limited to the range relatively close to the critical temperature and magnetic field. Furthermore, analyzing the system from a microscopic point of view is essential to understanding superconductivity on such a small scale. Latest experimental efforts aimed at STM imaging of mesoscopic vortex matter have focused on NbSe₂ samples [20], since direct STM images of vortex states have been obtained only on high-quality single crystals of NbSe₂ [21] and Bi₂Sr₂CaCuO_{8+δ} [22–24]. These compounds are highly two-dimensional and easy to cleave *in situ*, providing very clean surfaces – a key ingredient for successful STM imaging. Thus, anticipating STM measurements, we present in this paper self-consistent BdG results with parameters corresponding to submicron NbSe₂ disks.

II. FORMULATION

We consider an *s*-wave superconducting disk of radius R under a magnetic field perpendicular to the disk area, with a vortex carrying m fluxoid quanta formed in the center. The system has cylindrical symmetry and it is described using cylindrical coordinates (r, θ, z) . In accordance with the experiments [6,20] we assume the disk thickness to be much smaller than the penetration depth. Consequently, the order parameter is assumed to be uniform in the field direction (\hat{z}), and the current density \mathbf{j} as well as the vector potential \mathbf{A} has no z component [7]. In the gauge which removes the phase of the order parameter [11], i.e., $\Delta(\mathbf{r}) = |\Delta(r)|$, we can write down the radial part of the BdG equations [25,13,26] as

$$\begin{aligned} & \sigma_z \frac{\hbar^2}{2m_e} \left[-\left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) \right. \\ & \left. + \frac{1}{r^2} \left\{ l - \sigma_z \left(\frac{e}{\hbar c} r \tilde{A}_\theta(r) + \frac{m}{2} \right) \right\}^2 \right] \hat{\psi}_n(r) \\ & + \sigma_z (U(r) - \mu) \hat{\psi}_n(r) + \sigma_x |\Delta(r)| \hat{\psi}_n(r) = \epsilon_n \hat{\psi}_n(r), \end{aligned} \quad (1)$$

where

$$\hat{\psi}_n(r) = \begin{pmatrix} u_n(r) \\ v_n(r) \end{pmatrix} \quad (2)$$

is the radial quasiparticle amplitude. Here σ_x and σ_z are the Pauli matrices, m_e is the electron mass, and μ the

switches is studied. This work discusses the tunneling density of states in the core of giant vortices in terms of quasiclassical calculations.

chemical potential. The angular momentum quantum number l is an integer when m is even, and a half odd integer when m is odd [11]. The single-particle potential $U(r)$ can incorporate the lattice potential and inhomogeneity effects due to impurities and sample boundaries. To study quantum size and interference effects, we consider a clean sample and take $U(r) = 0$ inside the disk, while including the periodic lattice potential in terms of the effective masses, m_r and m_z . Furthermore, we take $m_z \gg m_r$, as justified for highly anisotropic materials such as NbSe₂, and neglect the dependence of Eq. (1) on the motion along the z direction.

In principle, due to finite thickness of the sample, the vector potential must depend on not only r but also z , so that $\mathbf{A} = A_\theta(r, z) \hat{\theta}$, and $\tilde{A}_\theta(r)$ in (1) is an average of $A_\theta(r, z)$ over the disk height L [7]:

$$\tilde{A}_\theta(r) = \frac{1}{L} \int_{-L/2}^{L/2} dz A_\theta(r, z). \quad (3)$$

However, for typical experimental parameters [6,20] the lateral sample size is much larger than the thickness, and we therefore consider the case where the vector potential is independent of the z coordinate; $A_\theta(r, z) \simeq A_\theta(r)$. The order parameter and the current density $\mathbf{j} \equiv j_\theta(r) \hat{\theta}$ are given in terms of the eigenvalues and eigenfunctions of Eq. (1) as

$$\begin{aligned} |\Delta(r)| &= g \sum_{\epsilon_n \leq \hbar \omega_D} u_n(r) v_n^*(r) (1 - 2f_n) \quad (4) \\ j_\theta(r) &= \frac{e\hbar}{m_r r} \sum_n \left[\left(l - \frac{m}{2} - \frac{e}{\hbar c} r A_\theta(r) \right) |u_n(r)|^2 f_n \right. \\ &\quad \left. - \left(l + \frac{m}{2} + \frac{e}{\hbar c} r A_\theta(r) \right) |v_n(r)|^2 (1 - f_n) \right], \end{aligned} \quad (5)$$

where g is the coupling strength for the electron-electron attraction, ω_D is the Debye frequency, and $f_n \equiv f(\epsilon_n)$ is the Fermi distribution function. The vector potential is given in turn by the current density through the Maxwell equation $\nabla \times \nabla \times \mathbf{A} = (4\pi/c) \mathbf{j}$. We first solve Eq. (1) with initial guesses for $|\Delta(r)|$ and $A_\theta(r)$ and recalculate them from Eqs. (4) and (5), and repeat the process until self-consistency is acquired. The local tunneling density of states and the differential conductance [25,13] can then be calculated by

$$\begin{aligned} N(r, E) &= \sum_n [|u_n(r)|^2 \delta(E - \epsilon_n) \\ &\quad + |v_n(r)|^2 \delta(E + \epsilon_n)] \quad (6) \\ \frac{dI(r, V)}{dV} &\propto - \sum_n [|u_n(r)|^2 f'(\epsilon_n - eV) \\ &\quad + |v_n(r)|^2 f'(\epsilon_n + eV)]. \end{aligned} \quad (7)$$

Clearly, the differential tunneling conductance (7) is a direct probe of the local density of states, $N(r, E)$, pro-

vided that the temperature is low enough. In the following we will present some results for the experimentally observable differential conductance at low temperatures, but may refer to it as the local tunneling density of states (LDOS). We choose the parameters corresponding to NbSe₂: we take $m_r = 2m_e$, $E_F = 37.3$ meV, $\hbar\omega_D = 3.0$ meV, and set the coupling strength so that the bulk gap $\Delta_0 \equiv 1.12$ meV.

The results are shown for disk radius $R = 500$ nm. We have investigated the size range of $R = 200 - 600$ nm and have found qualitatively same features in the LDOS.

III. RESULTS

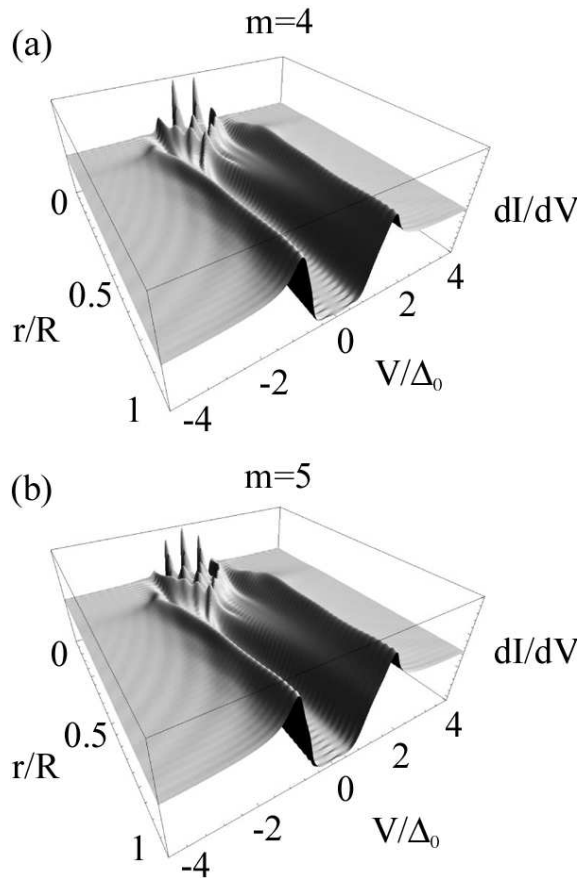


FIG. 1. Local tunneling conductance as a function of coordinate r and voltage V , for a giant vortex state with (a) $m = 4$ and (b) $m = 5$ flux quanta, sustained in a superconducting disk with radius $R = 500$ nm at temperature $T = 1$ K.

In Fig. 1 we show the differential conductance for a vortex with (a) $m = 4$ and (b) $m = 5$ flux quanta, as a function of voltage V and radial distance r from the

disk center, for temperature $T = 1$ K[†]. In both cases, prominent sharp peaks can be seen near the vortex core and for low voltages – four peaks in the former and five in the latter. Generally speaking, the number of low-bias conductance peaks corresponds to the winding number m of the order parameter, which gives rise to m peaks near the center [13,26]. This feature is in accordance with the index theorem established by Volovik [27] for the Caroli-de Gennes-Matricon bound states in a vortex core. According to this theorem, the quasiparticle spectrum of a vortex with winding number m has m branches of bound states, which cross zero energy as a function of angular momentum. These quasiparticle branches also explain the evolution of the m rows of conductance peaks as one moves away from the core, as seen in Fig. 1, with decreasing number of peaks one by one [13]. In contrast to the singly quantized case [28], one can see directly that as energy increases, more states with higher angular momenta contribute to the density of states.

We illustrate this in Fig. 2, where a spatial map of the LDOS is taken for various fixed values of V . Clearly, with increasing bias voltage the density of states is redistributed from the core towards the sample boundaries. Fig. 1 also reveals the presence of the so-called zero mode, i.e., a peak around zero energy at the vortex core for odd m , and its absence for even m . The existence of a zero mode is, quite generally, linked to a sign change in the order parameter as a function of some generalized coordinate [29]. The zero-bias peak is a signature of bound states for quasiparticles trapped by the sign change. Here, in the given gauge, the order parameter changes sign at the vortex core when m is odd, while it does not when m is even.

The low-bias peaks and zero modes discussed above are general characteristics of the LDOS associated with the winding number of the order parameter. In addition to these, however, we have found novel features in the LDOS that are unique to giant vortex states in sub-micron disks. They are the oscillations seen above the gap energy in Figs. 1 and 2(c) and more clearly in the contour plot of Fig. 3. These oscillations are similar in origin to the so-called Tomasch oscillations discovered in a superconductor-normal metal junction [30–32] and reflect “standing waves” arising from the interference of quasiparticle states. This interference effect is a direct consequence of strong confinement experienced by the superconducting quasiparticles due to the small system size. We dedicate the remainder of this paper to detailed discussions of this effect.

[†]For data to be shown for energies well above the gap energy, fast $1/k_F$ oscillations have been removed by means of Fourier transform. In actual observations these fast oscillations will not be resolved.

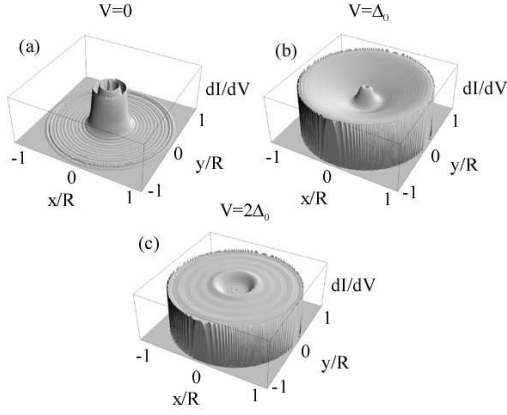


FIG. 2. Spatial map of the local tunneling conductance for the entire disk in the giant vortex state of Fig. 1(b), for various fixed voltages. It can be seen that the maxima in the local density of states gradually shift towards the perimeter of the disk as the voltage is increased.

When a vortex holds multiple flux quanta m , the order parameter vanishes around the center over a certain area – the larger the m is, the larger the area [26]. As the distance from the center increases, the order parameter increases and recovers to its bulk value eventually. In the case of NbSe₂, due to the short coherence length, the recovery happens relatively quickly. This results in a well-defined superconducting region with the constant order parameter Δ_0 within the disk. At the disk boundaries, however, the order parameter is forced to vanish and as a result, exhibits Friedel-like oscillations around its bulk value near the surfaces. These oscillations have the largest amplitudes at the boundaries and decay roughly over the coherence length scale. Moreover, the smaller the system size, the larger these amplitudes relative to the bulk value. The quasiparticles confined in the disk experience scattering by this large change in the order parameter at the surfaces. An electron-like quasiparticle is reflected back as a hole-like one and vice versa, and the Tomasch effect results from the interference between the electron-like and hole-like states in the superconducting region [32]. The momenta of electron-like and hole-like quasiparticles for energy E are $k^\pm = \frac{\sqrt{2m_r}}{\hbar} \sqrt{E_F \pm \Omega} \simeq k_F \pm \frac{\Omega}{\hbar v_F}$, respectively, where $\Omega = \sqrt{E^2 - |\Delta(r)|^2}$ with $|\Delta(r)| \simeq \Delta_0$ and k_F is the Fermi momentum. At a given distance d from the surface, the LDOS oscillations in energy are determined

by [32] $\frac{E_n}{\Delta_0} \simeq \sqrt{1 + n^2 \left(\frac{\pi \hbar v_F}{\Delta_0 d} \right)^2}$, where n is an integer, and $\frac{\pi \hbar v_F}{\Delta_0} \simeq 151.15$ nm for NbSe₂. Furthermore, the interference can be seen in the LDOS also as a function of coordinate (distance from the surface) for a given energy E . The period of the oscillations in this case is given by $\delta d \simeq \frac{\pi \hbar v_F}{\Delta_0} \frac{1}{\sqrt{(E/\Delta_0)^2 - 1}}$. The oscillation periods obtained in our numerical results, as seen in Fig. 3,

are in quantitative agreement with these analytical expectations.

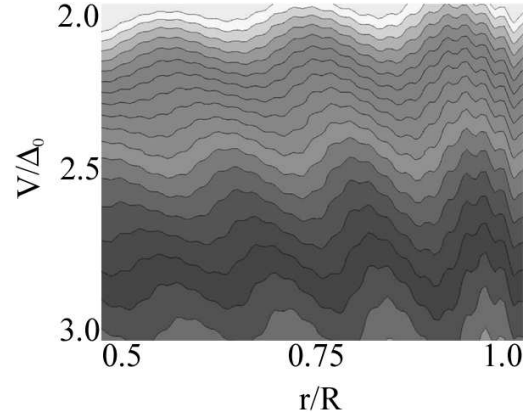


FIG. 3. Contour plot of the LDOS in Fig. 1(b) in the superconducting region, where the Tomasch density of states oscillations occur.

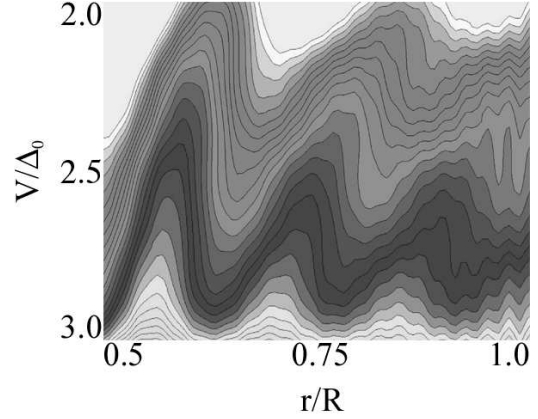


FIG. 4. Same as Fig. 3, but for the corresponding model calculation.

In a superconductor with short coherence length, if the winding number m and, consequently, the “normal core” area is very large, the Tomasch effect may arise also from the vortex core, as in a normal-superconductor junction. For submicron NbSe₂ disks with m up to five, however, we have found that the LDOS is dominated by the Tomasch oscillations coming from the surfaces. Indeed, we have confirmed the LDOS oscillations characteristic of the Tomasch effect in terms of model calculations in one and two dimensions, where the BdG equations are solved without iteration with a step-function order parameter: $\Delta(r) = 0 (r < R/2); \Delta_0 (r > R/2)$. In this case the Tomasch effect coming from the normal-superconductor interface governs the LDOS structure, so that the oscillation period in energy (see E_n above) becomes larger as one approaches the interface (i.e., here d is the distance from the interface). Apart from this and enhanced amplitudes due to a larger change in the

order parameter, the LDOS shows the same qualitative features as seen above (compare Figs. 3 and 4).

IV. CONCLUSIONS

We have presented detailed, self-consistent calculations of the microscopic electronic structure of giant vortex states. We believe that the most direct experimental evidence for the existence of giant vortices can be provided by STM measurements of the local density of states in sub-micron superconductors capable of sustaining such vortex configurations. We have provided a spatial map of the tunneling density of states for multi-quantum giant vortex states, and have identified several signatures that can be used to identify them with STM. We have found that under extreme confinement the quantum interference arises among quasiparticle states and leads to experimentally observable Tomasch oscillations in the local density of states.

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